Spectroscopy for Industrial Applications: High-Temperature Processes

Fateev, Alexander; Grosch, Helge; Clausen, Sønnik; Barton, Emma J.; Yurchenko, Sergei N.; Tennyson, Jonathan

Publication date:
2014

Document Version
Publisher's PDF, also known as Version of record

IV-5. Spectroscopy for Industrial Applications: High-Temperature Processes

Alexander Fateev[a], Helge Grosch[a], Sonnik Clausen[a], Emma J. Barton[b], Sergei N. Yurchenko[b], Jonathan Tennyson[b]

[a] *DTU Chemical Engineering, Frederiksborgvej 399, DK-4000, Roskilde, Denmark*

[b] *Department of Physics and Astronomy, University College London, London WC1E 68T, UK*

The continuous development of the spectroscopic databases brings new perspectives in the environmental and industrial on-line process control, monitoring and stimulates further optical sensor developments. This is because no calibration gases are needed and, in general, temperature-dependent spectral absorption features gases of interest for a specific instrument can in principle be calculated by knowing only the gas temperature and pressure in the process under investigation/monitoring. The latest HITRAN-2012 database contains IR/UV spectral data for 47 molecules and it is still growing. However use of HITRAN is limited to low-temperature processes (< 400 K) and therefor can be used for absorption spectra calculations at limited temperature/pressure ranges. For higher temperatures, the HITEMP-2010 database is available. Only a few molecules CO_2, H_2O, CO and NO are those of interest for e.g. various combustion and astronomical applications are included. In the recent few years, several efforts towards a development of hot line lists have been made; those have been implemented in the latest HITRAN-2012 database[1].

High-resolution absorption measurements of NH_3 (IR, 0.1 cm^{-1}) and phenol (UV, 0.019 nm) on a flow gas cell[2] up to 800 K are presented. Molecules are of great interest in various high-temperature environments including exoplanets, combustion and gasification. Measured NH_3 hot lines have been assigned and spectra have been compared with that obtained by calculations based on the BYTe hot line list[1]. High-temperature NH_3 absorption spectra have been used in the analysis of in situ high-resolution IR absorption measurements on the producer gas in low-temperature gasification process on a large scale. High-resolution UV temperature-dependent absorption cross-sections of phenol are reported for the first time. All UV data have been calibrated by relevant GC/MS measurements. Use of the data is demonstrated by the analysis of in situ UV absorption measurements on a small-scale low-temperature gasifier. A comparison between in situ, gas extraction and conventional gas sampling measurements is presented. Overall the presentation shows an example of successful industrial and academic partnerships within the framework of national and international ongoing projects.

[1] S.N. Yurchenko, R.J. Barber and J. Tennyson "A variationally computed hot line lists for NH_3", MNRAS, 413, 1828-1834 (2011).

[2] H. Grosch, A. Fateev, K.L. Nielsen and S. Clausen "Hot gas cell for optical measurements on reactive gases", JQSRT, 130, 392-399 (2013).